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Exascale Computing Challenges for Energy Harvesting Systems

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Abstract. We develop massively parallel, extreme-scale, open-source codes, based on advanced, high-order numerical algorithms targeting production runs on exascale architectures. We conduct simulation-based investigations for science problems in predicting the optical, electrical, mechanical, thermal properties for complex systems in energy applications. The successful outcome of our works will benefit a wide range of relevant research communities and industries in the production of plasmonic devices, photovoltaic cells, electronic and storage devices, batteries, semiconductors, fuel cells, water reactors, etc.

Computational Approaches. Our algorithms and software development focus on efficiently and accurately solving Maxwell, Schrödinger, drift-diffusion, and lattice Boltzmann equations. We consider high-order spectral element discretization discontinous Galerkin (SEDG) discretizations based on the Nth-order tensor product of one-dimensional Lagrange interpolation polynomials using the Gauss-Lobatto-Legendre grid points with explicit-type time-advancing scheme whose computations involve mainly matrix-vector multiplications. Our mass matrix is fully diagonal with no additional cost for mass matrix inversion. For the communication, the data exchange only occurs between face to face. Messages between element faces are stored into a single array for all the field components and communicated only one time per time step to minimize the communication latency.

Exascalable Solvers. Extreme-scale computing platforms featuring more than 10^9 cores and supporting world-leading computing infrastructure are DOE mission-critical projects. Enabling simulation-based investigation on such platforms will advance scientific understanding of complex systems that are too large for experimental study and will reduce both the time and the cost of prototyping and deploying new technologies. To this end, we develop software packages, NEKCEM and NEKLBM, for solving electromagnetics and fluids problems towards extreme-scale computing.

Performance and Scalability for Computation and I/O: We significantly improved in scalability and peak performance of the codes, NekCEM and NekLBM. We achieved 90% efficiency with 10% peak on Intrepid with 131072 cores and 60% efficiency on Jaguar with 262144 cores [1]. We developed scalable I/O algorithms, based on collective I/O, reduced-blocking I/O, and threaded reduced-blocking I/O. Threading approach achieves write bandwidth of 72 GB/s and 50 GB/s on 32,768 cores on BG/P and Cray XK 6, respectively, and greatly improves the production performance by overlapping the I/O latency with computation [2].

MPI vs. MPI+Threads: To achieve scalable performance with minimal parallelization overhead on multicore architectures, we have explored incorporating multithreading frameworks based on MPI/OpenMP and MPI/CUDA implementations, into our existing MPI codes, for intranode operations of MPI programs around time-consuming loops that do not contain data dependencies, while leaving the source code unchanged. Some prelimiary results are demonstrated in [3,4], showing speedup consistently when reducing MPI communication, increasing the number of threads, and having enough work for the compute-intensive sections.

Applications. The key components in developing scalable algorithms and software are based on high-order discretizations that deliver highly accurate solutions for predicitng physical quantities of complex systems on future extreme-scale platforms.

Scattering, Absorption, Carrier Dynamics in Plasmonic Solar Cells: Metals support surface plasmons at optical wavelengths and have the ability to localize light to subwavelength regions.

The field enhancements that occur in these regions set the ultimate limitations on a wide range of nonlinear and quantum optical phenomena. We consider both the classical and the quantum descriptions for free electron response inside metallic structures and apply the models to various geometries of film-coupled nanoparticles in plasmonic devices [5]. We also consider Schroödiger and drift-diffusion models to study the interplay between the absorption and current-generating characteristics of the materials combined with carrier production. Those models are constructed in NekCEM using the SEDG discretization approaches [6]. The accuracy and validation of these models are to be tested for a simple structure of plasmonic-based solar cell devices.

High-Order Lattice Boltzmann Methods for Turbulent Flows and Heat Transfer: We developed high-order SEDG lattice Boltzmann methods (LBM) and performed turbulent flow simulations and heat tansfer such as flow past a hemisphere, Kida flow, turbulent channel flow, natural convection flow, etc [7,8,9]. LBM is a mesoscopic approach that can describe the evolution of a single particle distribution function and its interaction with other particles. In our SEDG-LBM approach, we split the scheme into collision and streaming step and the SEDG discretization is applied to the streaming step of lattice Boltzmann equation after the collision step. For heat transfer simulations, we developed a thermal LBM model where the temperature is modeled with the macroscopic energy equation. We validate our schemes in comparion to the results by the Navier-Stokes solver Nek5000. We will ultimately use the methods for studying multiphase flows, including boiling phenomena for water reactor problems.

Future Works. Efficient and accurate predictive modleing will be performed for theoretical and experimental validation. Scalable algorithms will be developed and interagted into the software packges, NekCEM and NekLBM, to ensure good performance and scalability at exascale computing architecutre. These works involves cross-disciplinary research, strongly tied with my existing partneships and collaborations The resultant codes will enable highly efficient and accurate predictive modeling, with significant reduction in both the cost and the risk in the design process for energy applications.

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